WE CLAIM:

1. A computer-assisted method for determining a three-dimensional structure of a target amino acid sequence using a computer comprising a processor configured to receive and output data in accordance with executable code, the method comprising:

(a) generating input data for the computer comprising:

(i) inputting into the computer an alignment of a target amino acid sequence with a template amino acid sequence; and

(ii) by way of executable code, directing the processor to produce from the alignment a three dimensional reduced protein model comprised of representations of side chains of amino acid residues comprising a target protein; and

(b) outputting the three-dimensional reduced protein model to an output device or a storage device.

2. A method according to claim 1 wherein the executable code comprises instructions for:

(a) converting representations of the side chains of amino acid residues of the target protein to interaction centers connected by virtual covalent bonds, wherein each interaction center comprises a pseudoatom representing a center of mass of the side chain of the represented amino acid to which the interaction center corresponds, and wherein each interaction center, except for the interaction centers representing the amino and carboxy terminal amino acid residues of the target protein, is connected to an immediately proximal interaction center and an immediately distal interaction center via a virtual covalent bond to produce an interaction center chain; and

(b) projecting the interaction center chain onto an underlying cubic lattice to produce a projected chain of interaction centers;

(c) applying secondary constraints and/or tertiary constraints to a subset of interaction centers of the interaction center chain so as to produce a data set representing a three-dimensional model structure of the target protein.

3. A method according to claim 2 further comprising iterating steps (a)-(c), wherein in each iteration, a different set of secondary and tertiary constraints are applied to the interaction centers to produce a series of data sets representing three-dimensional model structures of the target protein, and wherein an energy computation is made for each member of the series of data sets representing the three-dimensional model structures of the target protein.

4. A method according to claim 3 further comprising selecting the member of the series of data sets representing the three-dimensional model structures of the target protein that has the lowest energy.

5. A method according to claim 4 wherein the data set representing the three-dimensional model structure of the target protein having the lowest energy is output to the data storage system to produce a stored data set.

6. A method according to claim 4 wherein the data set representing the three-dimensional model structure of the target protein having the lowest energy is output to an output device.

7. A method according to 5 wherein the stored data set is retrieved and displayed on an output device in a manner that allows the three-dimensional model structure of the target protein to be visualized.

8. A method according to claim 1 wherein the threading alignment input into the computer is retrieved from a data storage system.

9. A computer-assisted method for determining a three-dimensional structure of a target protein using a computer comprising a processor configured to receive and output data in accordance with executable code, the method comprising:

(a) generating input data for the computer comprising:

(i) inputting as a string of an identity constraint and a secondary structure constraint and/or tertiary constraints for some or all of the amino acid residues residue comprising the target protein; and

(ii) by way of executable code, directing the processor to produce from the string a three dimensional reduced protein model comprised of representations of side chains of the amino acid residues comprising the target protein; and

(b) outputting the three dimensional reduced protein model to an output device or a storage device.

10. A method according to claim 9 wherein the secondary structure constraint for each amino acid residue is selected from the group of "H" for helix, "E" for extended, and "(-)" for other structural constraints.

11. A method according to claim 9 wherein the secondary structural constraint for a subset of amino acid residues comprising the target protein is generated by a threading alignment of an amino acid sequence of the target protein.

12. A computer-assisted method for determining a three-dimensional structure of a target amino acid sequence, the method comprising inputting into the computer an alignment of a target amino acid sequence with a template amino acid sequence and calculating with the said computer one or more three-dimensional reduced protein model comprising representations of side chains of amino acid residues comprising a target protein.

13. A method according to claim 12 further comprising outputting to an output device or a storage device one or more of the three-dimensional reduced protein models.